A continuum consistent particle method for discrete fracture events and phase transformations in silicon

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The numerical analysis of damage and fracture in complex materials remains a challenge. Discrete particle methods are an attractive computational methodology since they can easily accommodate complex and arbitrary discontinuities. The computational predictive capabilities of particle methods in capturing intricate fracture events of elastic-brittle materials, has been convincingly demonstrated in the literature. Beyond linear elasticity and the small strain fracture regime, the ability of current particle methods such as the Discrete Element Method (DEM), Smoothed Particle Hydrodynamics (SPH) and Peridynamics to properly account for the underlying material behaviour remains problematic. Most of the discrete constitutive formulations are not providing results that are consistent with those obtained from true continuum simulations.

This contribution introduces an alternative particle-based formulation that relies on an appropriate averaging scheme that extracts the deformation gradient tensor at each particle based on the relative positions of the particle's nearest neighbours. The novel particle-based model, referred to as the Continuum Bond Method (CBM), preserves the constitutive properties of continuum methods while inheriting the powerful fracture properties of discrete particle methods. To illustrate this, two numerical examples are presented to reveal the achieved discrete-continuum consistency and its complex fracture capabilities: (i) an elasto-plastic tensile bar subjected to large deformations and (ii) a dynamic crack branching problem. In the first example, local and global mechanical responses obtained with CBM are assessed in direct comparison with a finite element continuum reference solution and further compared to discrete SPH results. The second numerical example exposes the CBM's capability to reproduce complex fracture events, which are driven by the elastodynamics in the simulation.

The particle-based CBM method is next extended for the micro-scale scratching of mono-crystalline silicon, where emphasis is put on the phase transformations. Two ingredients are important for this model: (i) a three-dimensional CBM implementation in LAMMPS and (ii) a proper constitutive model that describes the pressure-induced phase transformations in silicon (based on Budnitzki et al., 2012), here extended to finite strains). The resulting LAMMPS-CBM scratch setup is used to assess the response from the underlying model that phenomenologically captures silicon phase transitions under contact and scratch conditions. Comparisons are made with nano-scratch experiments carried out on silicon.

References

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